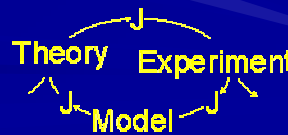


PySCeS

Python Simulator for Cellular Systems

Johann Rohwer, Brett Olivier, Jannie Hofmeyr

Triple-J Group for Molecular Cell Physiology
Stellenbosch University, South Africa



Modelling software Criteria

- **Accessible:** not limited to an operating system
- **Flexible:** modifiable and extendable
- **Functional:** combine the features we like



www.python.org



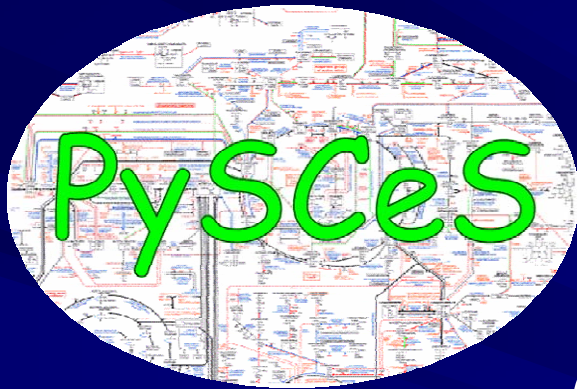
Python

- Modern object oriented programming language
- Free and available on many operating systems
- Interpreted scripting language
- It is easily extendable using C/C++/Fortran libraries

SciPy

- Open source library of scientific tools
- Integration and optimization routines
- BLAS, LAPACK, ATLAS
- Graphics and plotting modules
- Active user community

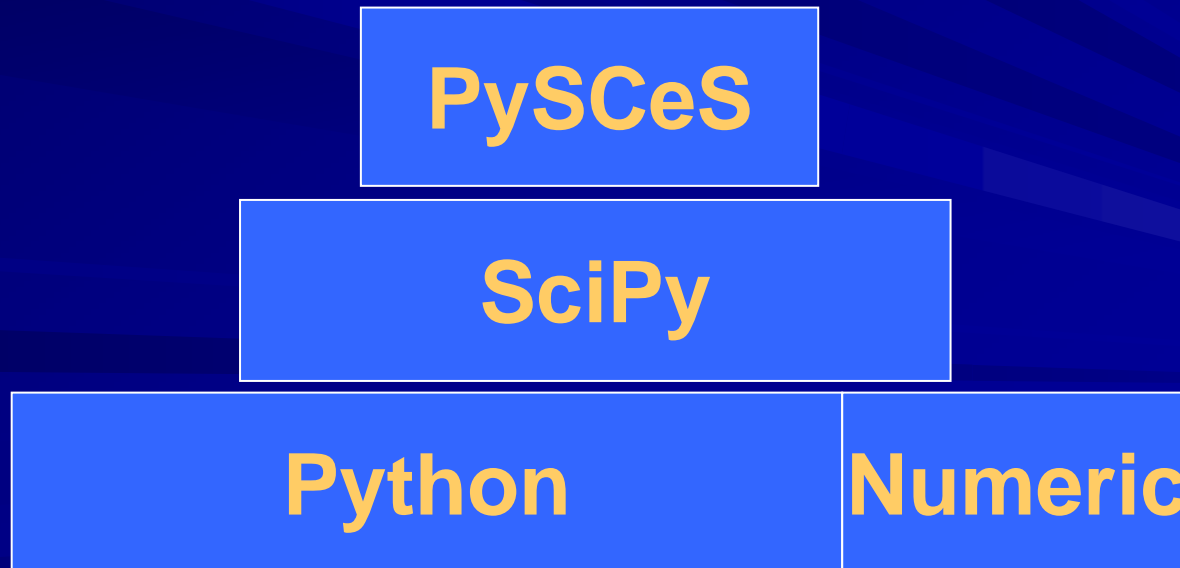
Python Simulator for Cellular Systems



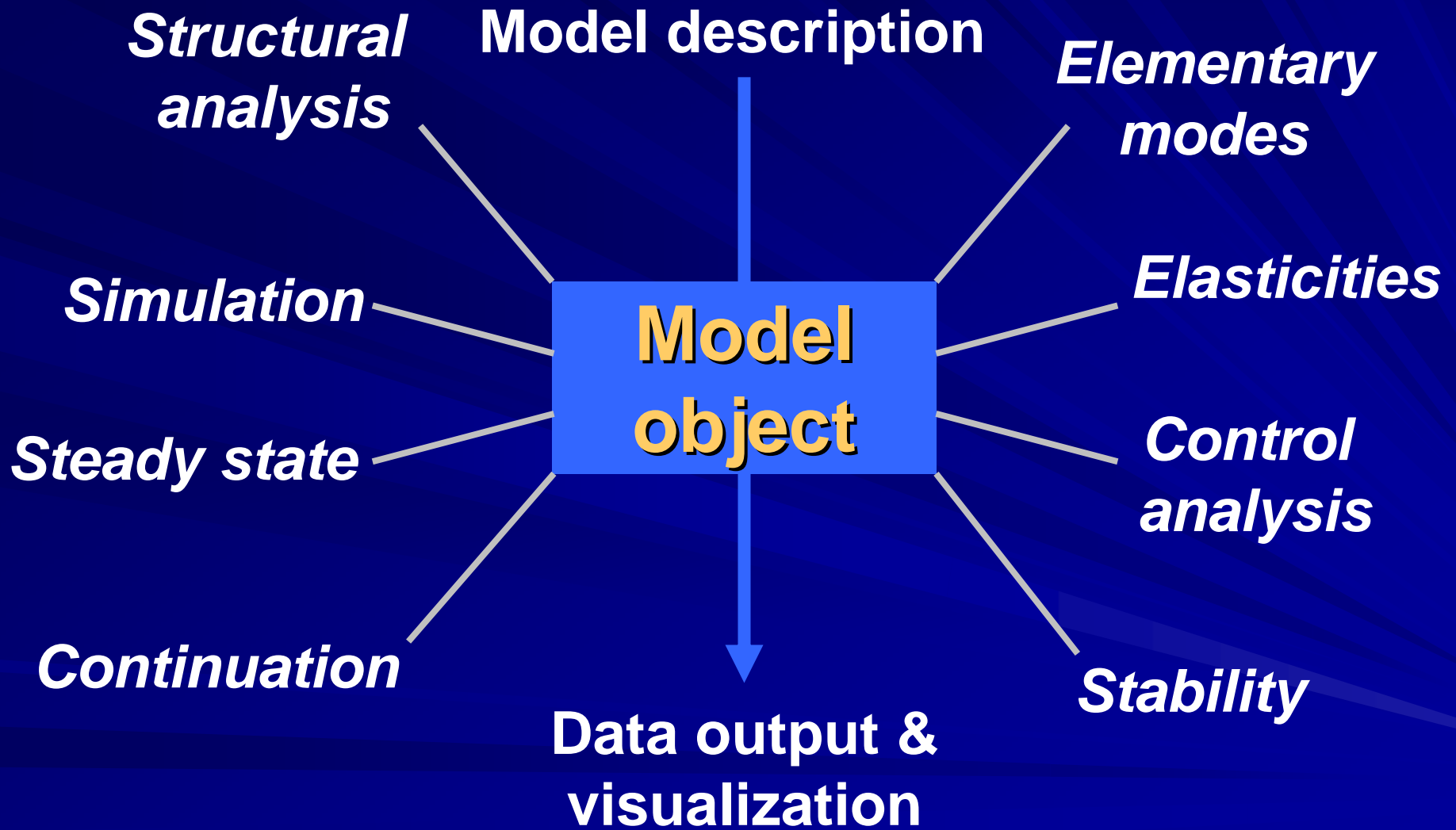
<http://pysces.sourceforge.net>



(GNU GPL licensing)



PySCeS



Starting PySCeS

```
Python 2.3.2 (#49, Oct 2 2003, 20:02:00) [MSC v.1200 32 bit (Intel)]  
Type "copyright", "credits" or "license" for more information.
```

```
IPython 0.6.3.cvs -- An enhanced Interactive Python.
```

```
>>> import pysces
```

```
pysces.PyscesModel.model_dir = /home/bgoli/pysces
```

```
pysces.PyscesModel.output_dir = /home/bgoli/pysces
```

```
*****
```

```
* Welcome to PySCeS (0.1.4) - Python Simulator for Cellular Systems*
```

```
* Copyright(C) Brett G. Olivier,2004 - http://pysces.sourceforge.net *
```

```
* Co-developed with J.-H.S. Hofmeyr and J.M. Rohwer *
```

```
* Triple-J Group for Molecular Cell Physiology *
```

```
* PySCeS is distributed under the GNU general public licence *
```

```
* See README.txt for licence details *
```

```
*****
```

```
>>>
```

Model properties

Model properties

```
>>> mod.x1
10.0

>>> mod.metabolites
('S2', 'S1', 'S3')

>>> mod.s1
5.0

>>> mod.Reaction1(mod)
0.2

>>> mod.Reaction1r
k1*x1 - k2*A
```

Structural Analysis*

```
>>> mod.lmatrix
array([[ 1.,  0.],
       [ 0.,  1.],
       [-1.,  0.]])

>>> mod.showK()
Kernel matrix (K)
      R3   R4
R3    1.0  0.0
R4    0.0  1.0
R1    1.0  1.0
R2    1.0  1.0

>>> mod.showConserved()
Conserved relationships
+ {1.00}S2 + {1.00}S3 = 1.0
```

Solving for the steady state

- Three solvers
 - HYBRD (modified Powell hybrid method)
 - NLEQ2 (affine invariant damped Newton)
 - Forward integration
- automatic switching (fallback)

```
>>> mod.doState()
(hybrd) The solution converged.
```

```
>>> mod.showState()
Steady-state metabolite concentrations
S2ss = 9.4882e-001
```

```
Steady-state fluxes
JR1 = 2.4343e-001
```

```
>>> mod.JR1
2.4343e-001
```

Data output

- showX(File) -- write information to screen or file
 - showN(), showNr(), showODE(), showEigen()
- Write_array_(arr) -- write arrays to file
 - Text, LaTeX, HTML
- pysces.plt.*
 - plot2D(arr), plot3D(arr)
- pysces.html.* -- html tags
 - par(str), h1(str)

Control coefficients				
	vfout	vgp	vpglm	vpgi
vfout	0.000	-0.000	-0.000	-0.000
vgp	0.000	-0.000	-0.000	-0.000
vpglm	0.000	-0.000	-0.000	-0.000
vpgi	0.000	-0.000	-0.000	-0.000
vpfk	0.000	-0.000	-0.000	-0.000
vald	0.000	-0.000	-0.000	-0.000
vtpi	0.000	-0.000	-0.000	-0.000
vgapdh	0.000	-0.000	-0.000	-0.000
vpgk	0.000	-0.000	-0.000	-0.000

Parameter continuation

- Uses PITCON (www.netlib.org)
- Can be used to investigate systems that have multiple steady states
- Implemented as a parameter scan

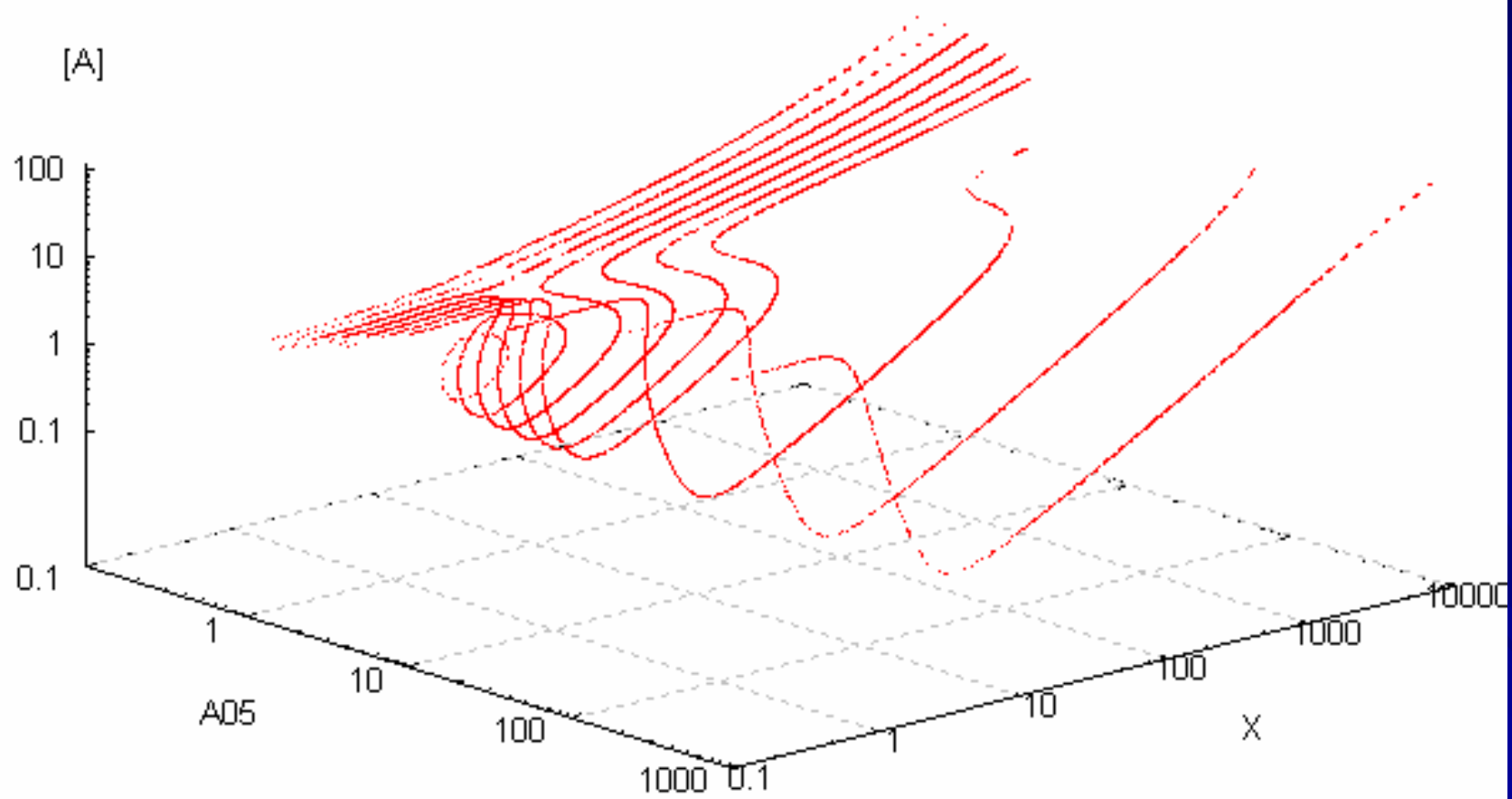
```
>>> mod.pitcon_par_space = scipy.logspace(-1,3,20)
```

```
>>> res = mod.PITCON('X')
```

```
>>> pysces.plt.plot2D(res, 0, [1,2], ykey=['A','B'], fmt='w p', log=1)
```

```
>>> pysces.plt.xlabel('X'); pysces.plt.ylabel('Concentration')
```

```
>>> pysces.plt.save_html('isola')
```



view: 56.0000, 48.0000 scale: 1.00000, 1.00000

Steady state concentration of **A** plotted against a change in parameter **X** at different values of **$A_{0.5}$**

Summary

- **Python/SciPy** is a flexible environment for scientific computing
- **PySCeS** is being actively developed as a flexible modelling tool (current version -- 0.1.3)
- Current priority: **SBML** integration

Acknowledgements

Lead developer: Brett Olivier

SBML: Lafras Uys

Triple-J Group

Jannie Hofmeyr

Jacky Snoep

“Every good work of software starts
by scratching a developer’s itch.”

Eric Raymond (*The cathedral and the bazaar*)

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